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Theoretical Study of Oxygen Reduction Reaction (ORR) on Graphene and Pt-Supported Catalysts

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The global energy demand has risen sharply in recent decades due to population growth and increasing per-capita consumption. To achieve sustainable development and meet decarbonization goals, the transition toward clean and efficient energy conversion systems has become essential. Within this framework, the oxygen reduction reaction (ORR) plays a central role in electrochemical devices such as fuel cells and metal–air batteries, as highlighted by extensive experimental research on platinum-based catalysts[a].

However, the ORR is a kinetically sluggish process, requiring efficient catalysts to overcome its high activation barriers. Platinum remains the benchmark catalyst for this reaction, yet its scarcity and cost drive the search for more sustainable alternatives or configurations that enhance Pt utilization. Theoretical studies have provided critical insight into the origin of the ORR overpotential and the adsorption energetics of key intermediates[b]. In this work, a comparative theoretical study of pristine graphene (Gr) and Pt-doped graphene (Gr–Pt) was conducted under neutral and anionic conditions to evaluate their catalytic behavior toward the ORR.

Several intermediates were characterized along the reaction pathway, revealing distinct structural and electronic trends between both systems. Analytical tools such as the projected density of states (pDOS), differential charge density (Δρ), and Bader charge analysis provided insight into the interaction between oxygenated intermediates and the catalyst surface, as well as the effect of electronic injection on reaction energetics.

These results contribute to a deeper understanding of the structure–activity relationship in carbon-based and Pt-modified materials, offering valuable guidelines for the rational design of next-generation ORR catalysts and related electrochemical processes.

References:

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